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Realization of wide electron slabs by polarization bulk doping in graded III-V nitride semiconductor alloys

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Abstract

We present the concept and experimental realization of polarization-induced bulk electron doping in III-V nitride semiconductors. By exploiting the large polarization charges in the III-V nitrides, we are able to create wide slabs of high density mobile electrons without introducing shallow donors. Transport measurements reveal the superior properties of the polarization doped electron distributions than comparable shallow donor doped structures. The technique is readily employed for creating highly conductive layers in many device structures.

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Doping in semiconductors has been a much researched topic. The traditional shallow 'hydrogenic' doping technique is very well understood and gainfully employed. A good understanding of the role of ionized dopant atoms on carrier scattering in semiconductors led to the concept of modulation doping, which improved low temperature carrier mobilities in quantum-confined structures by many orders of magnitude [1].

The last decade witnessed the emergence of the III-V nitrides as a wide bandgap semiconductor with the property of large embedded electronic polarization fields owing to the lack of inversion symmetry in the crystal structure [2],[3]. This property has been widely exploited to make nominally undoped two-dimensional electron gases (2DEGs) in AlGaN/GaN heterostructures, which had led to high-electron mobility transistors (HEMTs) with record high performance characteristics[4]. The 2DEG at the AlGaN/GaN interface of a III-V nitride heterostructure is formed to screen the polar-

ization dipole (with spontaneous and piezoelectric contributions) in the thin epitaxial AlGaN cap layer. Surface donor-like states act as modulation dopants, supplying electrons to form a dipole with the 2DEG at the heterointerface[5].

The discontinuity of polarization across an $Al_xGa_{1-x}N$/GaN heterojunction $\Delta P_{hj} = P_{tot}^{AlGaN}(x) - P_{Sp}^{GaN}$ forms a fixed polarization sheet charge at the heterojunction. Grading the AlGaN/GaN heterojunction over a distance should spread the positive polarization sheet charge into a bulk three-dimensional polarization background charge. The charge profile is given by the divergence of the polarization field, which changes only along the (growth)z-direction ($N_D^{Pol}(z) = \nabla \cdot P = \frac{\partial P(z)}{\partial z}$). This fixed charge profile will depend on the nature of the grading; a linear grade results in an approximately uniform profile given by $N_D^{Pol}(z) = \frac{P(z_0)-P(0)}{z_0}$. Here $P(z_0)$ is the polarization (spontaneous+piezoelectric) of $Al_xGa_{1-x}N$ at the local Al composition at $z = z_0$.

This fixed background charge attracts free carriers from remote donor-like states to satisfy Poisson's equation and charge neutrality. Figure 1 shows the schematic band diagrams and charge profile showing the effect of linear grading of the heterojunction. The end result of the charge rearrangements makes the polarization bulk charge act as a local donor with zero activation energy. The mobile three-dimensional electron slab (3DES) thus formed should be usable just as bulk doped carriers. However, removal of ionized impurity scattering should result in higher mobilities. Such polarization induced electron slabs should in principle be similar to the modulation doped three-dimensional electron slabs in modulation doped wide parabolically graded quantum wells in the AlGaAs/GaAs system [6]. The mobile 3DES should not freeze out at low temperature (as shallow donor doped bulk carriers do), and should exhibit high mobilities at low temperatures.

To verify these concepts, five samples were grown by molecular beam epitaxy (MBE). Active nitrogen was provided by a rf-plasma source. High resistivity semi-insulating (SI) GaN on sapphire grown by metal-organic chemical vapor deposition (MOCVD) was used as templates. For all five samples, a 100nm buffer MBE layer of undoped (Ga-face) GaN was grown, followed by a different cap layer for each. The cap layer for the five samples are described in Table I. The top 100nm of sample 1 is bulk shallow donor doped with Si (activation energy $E_D = 20meV$, and concentration $N_D = 10^{18}/cm^3$). Samples 2,3 and 4 are linearly graded AlGaN/GaN structures for studying polarization bulk doping; they are graded from GaN to 10%, 20% and 30% AlGaN re-

spectively over z_0=100nm. Sample 5 is a 20nm $Al_{0.2}Ga_{0.8}N$/GaN which houses a conventional 2DEG at the heterojunction. Samples 1 and 5 are control samples.

Triple-crystal X-Ray diffraction data around the GaN (00.2) peak of samples 1-4 is shown in Figure 2. The data points match very well with the theoretical solid curves[7] reflecting the high degree of control of Al composition and growth rate in MBE. Atomic force microscopy (AFM) of the sample surfaces revealed step-flow growth and fully strained graded AlGaN surfaces. Secondary Ion Mass Spectroscopy (SIMS) was performed on an extra graded AlGaN layer sample specifically grown for that purpose. The linearity of Al composition in the graded layer was revealed by SIMS to be very accurately controlled. It also revealed background oxygen concentration in the MBE GaN layer to be identical to the underlying MOCVD layer accompanied with a small increase in the AlGaN layers. Any background oxygen (which acts as a shallow donor in (Al)GaN) may provide a small amount of thermally activated carriers which can be frozen out at low temperatures.

Temperature dependent (20-300K) Hall measurements were performed on all the five samples. Table I shows room temperature and 30K Hall measurement data for all five samples. The table includes the free carrier density in the bulk GaN and polarization induced 3DES and 2DEG densities calculated by solving Schrodinger and Poisson equations self consistently for samples 2-5. The room temperature sheet conductivity $\sigma = qn\mu$ is also shown. Temperature dependent carrier densities and mobilities for samples 1,4,and 5 are plotted in Figure 3 for comparison. Carriers in the 0-30% graded AlGaN sample mimics the transport characteristics of modulation doped 2DEGs and 3DESs characterized by a lack of activation energy, leading to a temperature independent carrier density. Carriers in the bulk donor doped sample show the characteristic freeze-out associated with the hydrogenic shallow donor nature of Si in bulk GaN. A fit to theoretical dopant activation yielded an activation energy[8] E_D = 20 meV with a doping density (fixed by the Si flux in MBE) $N_D = 10^{18}/cm^3$. The activation energy of Si closely matches that reported by Gotz et. al [9]. 2DEG carrier mobilities (Sample 5) are higher than the shallow donor doped and polarization doped carriers both at room temperature and low temperatures.

The point of interest is the order of magnitude improvement of carrier mobility at low temperatures for the polarization doped 3DESs over comparable donor doped samples. In donor doped GaN, thermally activated carriers freeze out with lowering of

temperature leading to less energetic electrons and less effective screening. This causes severe ionized impurity scattering, lowering the mobility. However, the removal of ionized impurity scattering in the polarization doped structure, aided by the complete lack of carrier freezeout at low temperatures results in much improved mobilities. It is not clear yet what limits the low temperature mobility of polarization doped 3DESs. Alloy disorder scattering could be a strong candidate since the 3DES is housed in a linearly graded disordered alloy potential. There is also an improvement of low temperature mobility with increasing carrier density, which points towards possible Coulombic scattering from surface donors, charged dislocations, and background shallow impurities. Dislocation scattering in the polarization doped 3DES is also reduced at low temperatures as compared to donor doped carriers owing to the degenerate nature of 3DES carriers[10]. Scattering from disorder in microscopic dipoles forming the graded alloy polarization charge could also be a source of scattering[11]. The unanswered questions open up avenues for further work in transport of polarization doped 3DESs.

Of special interest to device engineers is the room temperature mobility, and especially the conductivity $\sigma = en\mu$. From Table I, we see that the room temperature charge-mobility product of the polarization doped 3DES (Sample 3) is more than *double* of that of the comparable donor doped sample (Sample 1). Further, the trend with increasing alloy composition suggests that the conductivity *increases* with increasing carrier density (got by either grading to higher aluminum composition for the same thickness, or decreasing the thickness for same grading composition). This trend has proved very useful for our design of high conductivity layers required in many device structures, especially in field effect transistors (FETs) and regrown ohmic contacts. The additional band-discontinuity achieved at a regrown polarization-doped AlGaN contact serves as an efficient hot-electron launcher from the source into the FET channel, reducing the transit times. The flexibility of polarization doping by grading (by controlling alloy composition and/or graded layer thickness independently) is an added attraction. An interesting extension would be the possibility of achieving polarization doped p-type carriers with higher mobilities by grading down from AlGaN for Ga-face III-V nitrides. This might solve the problems associated with the high activation energy of the commonly used acceptor (Mg) for GaN. Our work presents the first step towards realizing the proposed enhancement of base conductivity in AlGaN/GaN heterojunction bipolar

transistors by exploiting the strong electronic polarization properties of the III-V nitride semiconductors [12].

In conclusion, we have demonstrated that polarization fields can be engineered to achieve bulk doping as an attractive alternate doping technique in III-V nitride semiconductors. We demonstrate improved conductivity of polarization doped layers over comparable donor doped layers, and point out avenues where it may be gainfully employed.

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Table caption

Table I : Sample structures and Hall measurement data for the five samples.

Figure captions

Figure 1 : Schematic band diagram and charge profile of polarization bulk doping by spreading the heterojunction sheet charge into a bulk charge.

Figure 2 : Triple crystal X-Ray diffraction data (dots) and theoretical curve (solid line) for Samples 1-4 around the GaN (00.2) peak. The close agreement between theoretically predicted and experimentally measured values indicates well controlled MBE growth.

Figure 3 : Temperature dependent carrier sheet densities and mobility for a Polarization doped (Sample 4), Donor doped (Sample 1) and a 2DEG (Sample 5) structures. Note the improvement in mobility and the lack of carrier activation for the polarization doped electrons compared to the donor doped electrons.

TABLE I:

Sample	Cap layer	Hall sheet density(cm^{-2})			Hall mobility ($\frac{cm^2}{V \cdot s}$)		300K Conductivity
		Theory	30K	300K	30K	300K	($10^{-4}\Omega^{-1}$)
1	100nm Bulk Si doped GaN	-	$7.3 \cdot 10^{11}$	$7.0 \cdot 10^{12}$	139	329	2.3
2	100nm 0-10% lin. gr. AlGaN	$2.5 \cdot 10^{12}$	$2.0 \cdot 10^{12}$	$1.7 \cdot 10^{12}$	1441	386	0.7
3	100nm 0-20% lin. gr. AlGaN	$5.8 \cdot 10^{12}$	$4.9 \cdot 10^{12}$	$7.8 \cdot 10^{12}$	2556	598	4.7
4	100nm 0-30% lin. gr. AlGaN	$9.0 \cdot 10^{12}$	$9.1 \cdot 10^{12}$	$8.9 \cdot 10^{12}$	2605	715	6.4
5	20nm $Al_{0.20}Ga_{0.80}N$ / GaN	$7.7 \cdot 10^{12}$	$7.7 \cdot 10^{12}$	$7.8 \cdot 10^{12}$	5644	1206	9.4

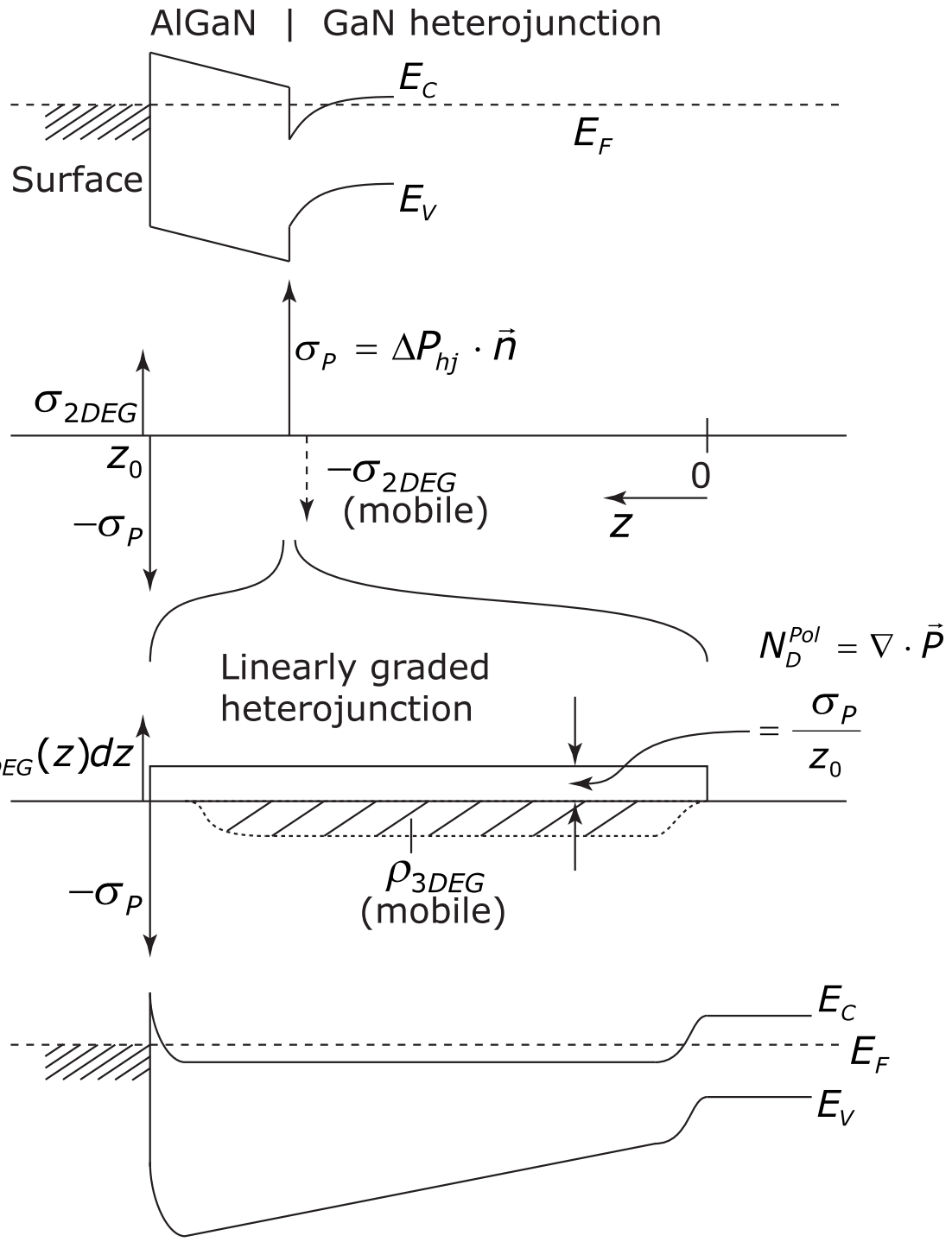

FIG. 1: (D. Jena *et. al.*)

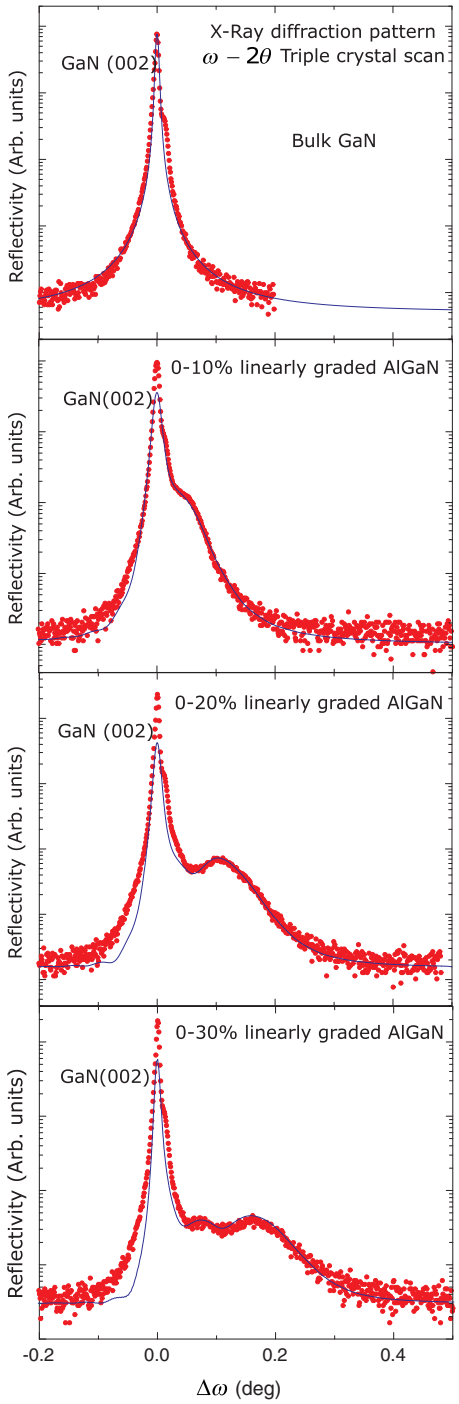

FIG. 2: (D. Jena *et. al.*)

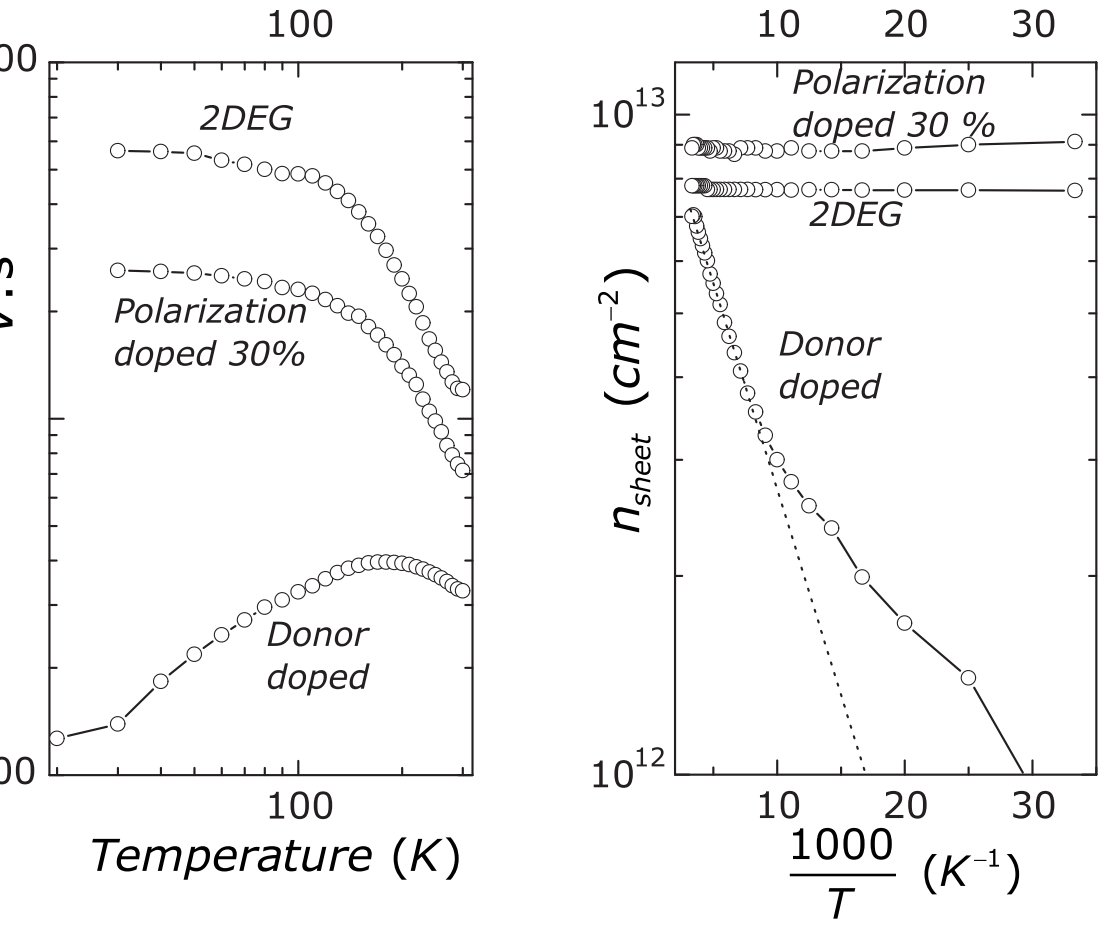

FIG. 3: (D. Jena *et. al.*)